



wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 4CF4
Title : Mutagenesis of a Rhodobacteraceae L-haloacid dehalogenase
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Deposited on : 2013-11-13
Resolution : 2.14 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

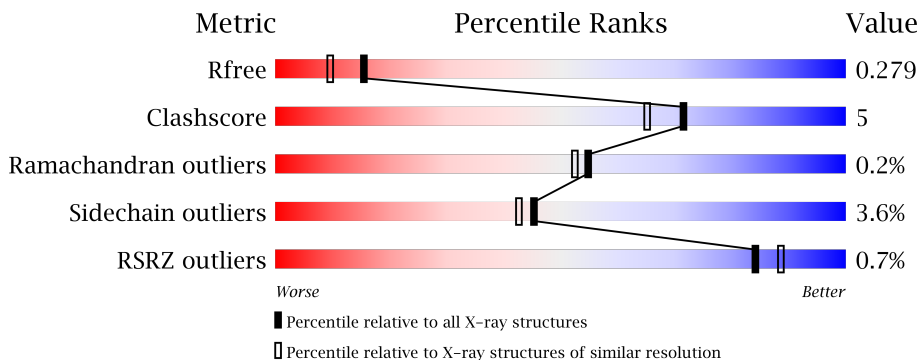
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	trunk24195
Percentile statistics	:	23426
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk24195

1 Overall quality at a glance

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	77520	1369 (2.16-2.12)
Clashscore	88313	1495 (2.16-2.12)
Ramachandran outliers	86584	1473 (2.16-2.12)
C α geometry	86677	1470 (2.16-2.12)
Sidechain outliers	86556	1473 (2.16-2.12)
RSRZ outliers	77580	1369 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	
1	B	236	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3578 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-HALOACID DEHALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1718	1103	288	321	6			
1	B	223	Total	C	N	O	S	0	0	0
			1718	1103	288	321	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	HIS	ENGINEERED MUTATION	UNP M9P6K0
B	183	HIS	HIS	ENGINEERED MUTATION	UNP M9P6K0

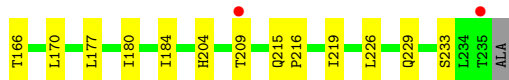
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	74	Total	O	0	0
			74	74		

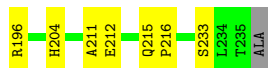
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• Molecule 1: L-HALOACID DEHALOGENASE

Age Group	Percentage
18-29	90%
30-49	86%
50-64	77%
65+	65%



Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.09Å 86.64Å 105.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.97 – 2.14 66.97 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.9 (66.97-2.14) 98.9 (66.97-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.202 , 0.280 0.201 , 0.279	Depositor DCC
R_{free} test set	1219 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 23766 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3578	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2114e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ASB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/1750	0.76	1/2390 (0.0%)
1	B	0.60	0/1750	0.75	0/2390
All	All	0.60	0/3500	0.76	1/4780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	LEU	CB-CG-CD2	-5.32	101.95	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1706	17	0
1	B	1718	0	1706	16	0
2	A	68	0	0	1	0
2	B	74	0	0	2	0
All	All	3578	0	3412	33	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:PRO:HG3	1:A:149:THR:HG21	1.66	0.78
1:B:129:SER:HB3	1:B:130:PRO:HD2	1.63	0.78
1:B:14:ILE:HB	1:B:177:LEU:HD23	1.78	0.66
1:A:14:ILE:HB	1:A:177:LEU:HD23	1.80	0.61
1:A:150:VAL:HB	1:A:155:ARG:O	2.05	0.56

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/236 (93%)	213 (97%)	6 (3%)	1 (0%)	36	29
1	B	220/236 (93%)	213 (97%)	7 (3%)	0	100	100
All	All	440/472 (93%)	426 (97%)	13 (3%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/193 (94%)	175 (96%)	7 (4%)	43	40
1	B	182/193 (94%)	176 (97%)	6 (3%)	48	47
All	All	364/386 (94%)	351 (96%)	13 (4%)	45	43

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	THR
1	A	233	SER
1	B	184	ILE
1	A	184	ILE
1	B	157	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	229	GLN
1	B	215	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ASB	A	18	1	9,11,12	4.96	2 (22%)	10,13,15	2.84	6 (60%)
1	ASB	B	18	1	9,11,12	4.39	3 (33%)	10,13,15	2.63	6 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ASB	A	18	1	-	0/8/11/13	0/0/0/0
1	ASB	B	18	1	-	0/8/11/13	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	ASB	C2-C1	14.28	1.51	1.49
1	B	18	ASB	C2-C1	12.47	1.51	1.49
1	A	18	ASB	OD1-CG	3.68	1.44	1.33
1	B	18	ASB	OD1-CG	3.14	1.42	1.33
1	B	18	ASB	CA-C	2.27	1.52	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASB	OD1-CG-CB	4.41	119.57	111.29
1	B	18	ASB	CA-CB-CG	-4.04	106.51	113.44
1	A	18	ASB	CA-CB-CG	-3.72	107.07	113.44
1	B	18	ASB	OD1-CG-CB	3.58	118.02	111.29
1	A	18	ASB	OD1-C2-C1	-3.56	101.25	108.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/236 (94%)	-0.39	3 (1%) 73 78	24, 43, 69, 111	0
1	B	223/236 (94%)	-0.32	0 100 100	25, 45, 78, 106	0
All	All	446/472 (94%)	-0.35	3 (0%) 84 88	24, 44, 76, 111	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	THR	2.4
1	A	131	ALA	2.2
1	A	235	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	ASB	A	18	12/13	0.10	1.48	25,33,39,40	0
1	ASB	B	18	12/13	0.08	-0.84	29,35,41,42	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.